

Process Evaluation and Optimization of Acetone Dehydration With Advanced Heat Integration Technology by the Techno-Economic Analysis

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ABSTRACT

Acetone refining processes are usually high in energy cost since the acetone purity and recovery rate should meet the product specification simultaneously. Different heat integration approaches are applied in a typical acetone refining process, which produce high-purity acetone product from crude acetone. The processes with energy-saving approaches are optimized according to total annual cost (TAC), and the TAC calculation results are compared to identify the energy-saving effects in the acetone refining process. Optimization is also applied for processes with different acetone product purity specifications to distinguish the influence of purity specification on final optimization results. The results showed that the heat integration can achieve a decrease of 30% on energy consumption and 17% on TAC, and the selection of product purity specification level also have an influence on energy cost and TAC. This indicated that the producers can vary their acetone product specification to obtain a large decrease of energy consumption according to their product purity demand, and it is also possible to use other separation methods with less energy cost in the treatment of acetone product with lower purity to improve the product purity, such as membrane separation.

Keywords: acetone, heat integration, separation, energy-saving, thermodynamic efficiency, CO₂ emission

NONMENCLATURE

Abbreviations

TAC	Total Annual Cost
CC/ C _p ⁰	Capital Cost
OC	Operating Cost

1. INTRODUCTION

Cumene hydroperoxide process is the most widely-used route for the production of phenol, which occupies 90% of the world's phenol production capacity. [1] Cumene hydroperoxide route is benefit for its advantages on low material cost, high product purity and the co-production of acetone product, but also constrained by its high energy cost. [2, 3] The energy consumption for the production of phenol and acetone in cumene oxidation process is mainly brought by the separation and purification, since a complex distillation sequence is required for the separation of reactants, products, byproducts and other unexpected impurities. [4]

The typical process has some disadvantages. The cumene reactant do not achieve a sharp separation in the crude acetone column, most of the cumene composition goes to the bottom of the crude acetone column mixed with phenol and other heavy components, which leads the separation in phenol purification section more complex. Decanter set at the bottom of the finished acetone separate the mixture as a water phase and a cumene phase. The water phase is treated as a waste water and is sent to sewer directly, which leads problems of waste water treatment and loss of reactant.

Also, the typical process cannot treat the mixture with higher methanol impurity. [2, 3, 5] The methanol impurity comes from the by-reaction of cumene and oxygen, and sometimes should be strictly controlled in the range of several hundred ppm in acetone product, such as in the production of bisphenol A. [6]

The purification in the finished acetone column is mainly a dehydration process, so it is also possible to consider the use of membrane or molecular sieve in acetone product purification, which may decrease the purity requirement of the distillation acetone product. Thus, it is also a possible approach to achieve energy savings via the decrease of acetone product purity by conventional distillation. The techno-economic research for the acetone refining section under lower acetone purities is of great importance. [7-9]

In this paper, a three-column process for acetone refining section in cumene hydroperoxide process is built and optimized via TAC analysis. Different methods of heat integration schemes are applied and compared. Processes with different product purities are also investigated to find the energy and cost saving potential with lower acetone product purities, with which the use of a membrane or molecular sieve can be taken into consideration.

2. PROCESS DESCRIPTION AND OPTIMIZATION

2.1 MODEL DESCRIPTION

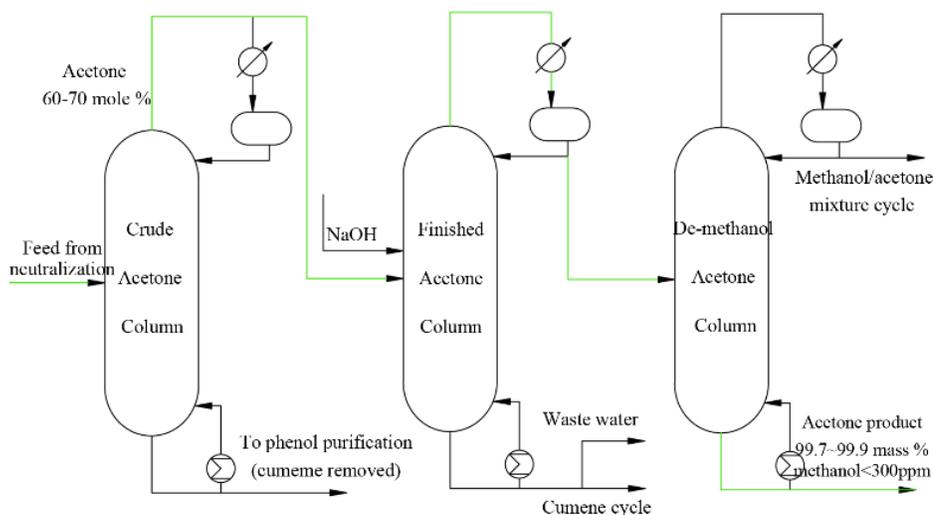
The detailed three-column acetone refining process model is shown in Fig.1. C1 is the crude acetone column, with a feed stream to be separated at the mid-part of the column. The feed composition is assumed as a mixture of

The determine of the feed composition ratio is based on real working conditions. C1 aims to remove all the components heavier than AMS (including phenol) from the light components. C2 aims to remove cumene and most of the water from the acetone product, and use NaOH aqueous to remove the trace amount of aldehyde. The top stream of C2 is sent to C3 for the de-methanol treatment. We specified the total acetone recovery rate as 99.5% in acetone product, and the methanol mass fraction should be lower than 300 ppm according to the acetone material standard for the production of bisphenol A. [10]

The rigorous model is set up in Aspen Plus using RadFrac module, and NRTL model is adopted for vapor-liquid equilibrium calculation. The binary interaction parameters are taken from the inner database of Aspen Plus, and the two pairs of losing binary interaction parameters (cumene/methanol and AMS/methanol) are estimated using UNIFAC method.

2.2 PARAMETER OPTIMIZATION

The optimization of process parameters is based on the cost and operation limits under actual working conditions. For the parameter determination in a distillation sequence, the first parameter that need to be decide is the operation pressures of columns, which is limited by the type of utilities, properties of the components to be separated, and energy and capital cost. It is highly recommended to use the atmosphere pressure as the operation pressure if possible, because the cost brought by pressure equipment or vacuum pump can usually be decreased. For the three-column



acetone, phenol, cumene, water, AMS and methanol.

process in this paper, the energy consumption is

Fig.1. Three-column acetone refining process model

influenced by operation pressure, and the variation trends of the three columns are shown in Fig.2. The energy consumption of C1 and C3 are not so sensitive to the operation pressure change, so the two columns are operated under atmosphere pressure. While with the operation pressure increase in C2, the energy consumption showed a sharp increase, which indicated that the separation in C2 is benefit from lower pressure. C2 is thus operated under vacuum condition. However, with the decrease of operation pressure, the top temperature of C2 is also decreased, which may lead the use of cooling water utility impossible.

An economic optimization procedure based on total annual cost (TAC) was applied to the three-column model to determine the other process parameters and achieve economic benefits. The calculation of TAC can be described in expression:

$$TAC = C_p^0 + OC/T$$

where C_p^0 (\$) is the capital cost (CC), OC (\$) is the operating cost, and T is the payback period, which was set as 5 years in this paper. The calculation model of TAC optimization was proposed by Turton et al. [11] and corrected using Chemical Engineering Plant Cost Index (CEPCI). [12] Details parameters and models about the TAC optimization are provided in the supporting file.

A sequential iterative optimization procedure was applied in the optimization process. [13] Considering there is no heat-integration or cycled stream in the typical process, the TAC optimization for each column is individual, and the overall sequential iterative optimization procedure need to be run for only once to find the optimized results.

The optimization results for the typical process are shown in Fig.3. The bottom temperature of C1 is higher than the temperature of LP steam or MP steam, so a HP steam utility is required for the C1 reboiler. C2 and C3 column use LP steam as heat source, and cooling water is applied for all the condensers.

3. HEAT INTEGRATION IMPROVEMENT

From the results in Fig.3, C1 is operated under high temperature and high temperature difference indicated that it is quite hard to use regular approaches on the decrease of C1 reboiler duty with the prevent distillation sequence. While considering the bottom temperature of C2 and C3, it is possible to achieve heat integration between C1 top vapor stream and C2/C3 bottom stream. On the other hand, considering a real working condition in a whole factory, there are usually waste hot water stream with a temperature of 70-80 °C that hard to be used in heat exchange. Assume the hot water stream as

80°C, it can be used as the heat source of C3. [14, 15] It is clear that the energy cost of C2 and C3 can be decrease enormously via such heat integration structure, while the small heat transfer difference required heat-exchangers with much larger heat transfer area, which obviously brings a capital cost increase. Thus, it is also necessary to apply the TAC optimization to processes with heat-integrated structures. [16]

Since the condenser duty of C1 is higher than the reboiler duty of C2, but lower than that of C3, and the hot water stream can only be used as the heat source of C3, seven different types of process with heat-integration structures were applied. To make the description convenient and clear, the seven integrated

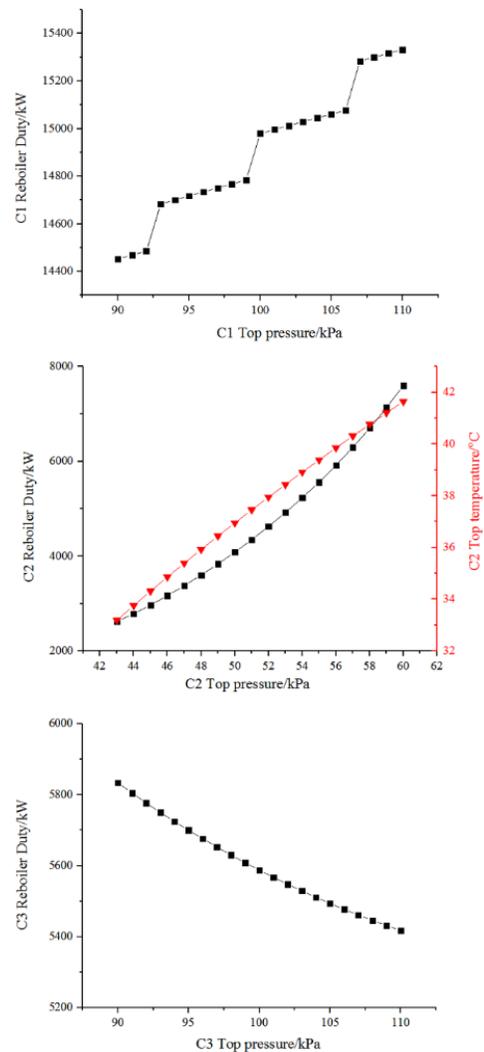


Fig.2. Energy consumption variation with different operating pressure

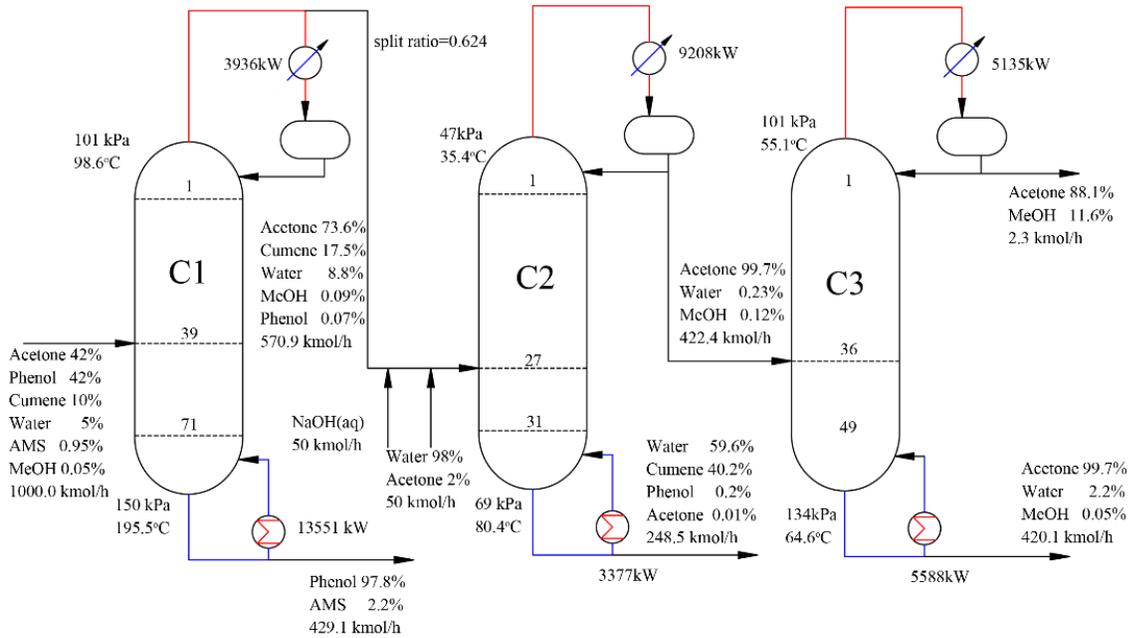


Fig.3. Optimization results for the typical process

process with the typical process are renumbered as followed, and the structures of all the eight processes are remark as S0a, S0b, S1a, S1b, S2a, S2b, S3a and S3b.

The TAC calculation for the heat-integrated structures has some differences compared with that of the typical process. Among the optimization we may reach a set of parameters that can achieve a nearly “full heat integration”, which means that the duty of trim-condenser or trim-reboiler is quite low or even 0, and all the reboiler duty can be supplied with C1 top vapor with no more condense duty required. [17] In fact, it is quite difficult to control a “full heat integration” process, so a trim-condenser/trim-reboiler with minimum heat transfer area of 10 m² is assumed then to ensure the controllability. [18-20] The heat integration structure leads an influence among the three columns, so the sequential iterative optimization procedure should be loop for several times until the parameters reach stable values. The operating cost of hot water is assumed as same price as cooling water, since the hot water are usually not utilized in the process as heat source. [14]

Fig.4 shows the cost comparison among the eight structures before and after optimization. For the cases that use the heat integration structure directly into the typical process, all the seven structures show higher capital cost compared with the typical structure. While if the heat integration structure is considered at the first beginning of the process design, which means that the structure parameters are optimized with heat integration structure concerned, the capital cost can be saved, and even lower than the typical process. The

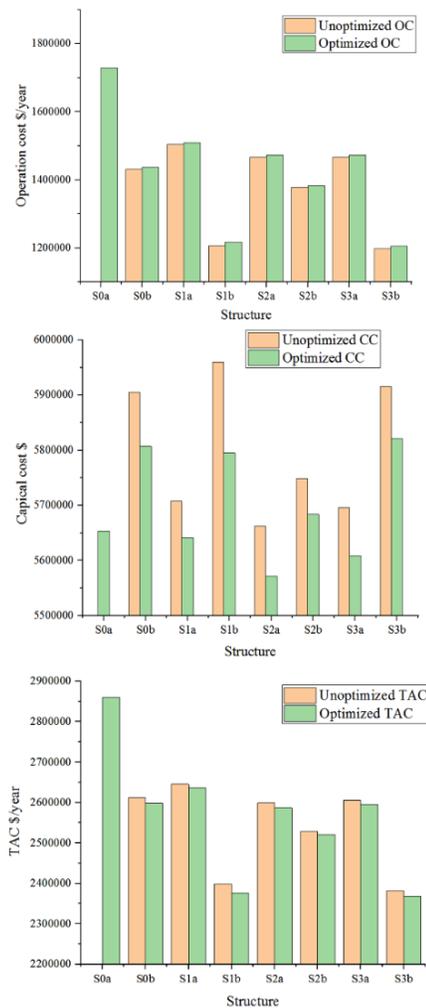


Fig.4 Cost of eight structures

energy consumption is decreased significantly in all the seven structures. S3b shows the largest energy saving with lowest TAC. S1b with simpler structure and similar energy/TAC saving percentage compared with S3b is also a suitable alternative structure.

4. STRUCTURES WITH DIFFERENT PRODUCT PURITY

The product purity of acetone product has two scales, the acetone mass fraction and the methanol mass fraction, which are set as 99.9% and 300 ppm in this paper, respectively. As we have talked in the introduction, it is possible to consider the use of membrane or molecular sieves in the acetone purification, and can decrease the purity requirement of the acetone product. The decrease of product purity can decrease the energy and capital cost in C2 and C3, and the cost saving levels is investigated in this section.

We first optimized two structures named S4 and S5 with acetone mass fraction as 99.8% and 99.7% respectively with methanol mass fraction unchanged, as shown in Table 1. The optimization result indicated that the decrease of acetone mole fraction leads a decrease of total energy consumption and capital cost, which is mainly contributed by C2. While this also increase the separation difficulty in C3, and the energy consumption and capital cost in C3 shows a small increase, which offset some cost saving.

Based on the process with lowest cost, two structures named S6 and S7 with methanol mass fraction as 400 ppm and 500 ppm respectively with acetone mass fraction with 99.7% is investigated and optimized, which also shown in Table 1.

Structure	S0a	S4	S5	S6	S7
CC \$	5653384	5469500	5407524	5117974	4878241
CC saving	0%	3.25%	4.35%	9.47%	13.71%
OC \$/year	1728896	1679454	1667202	1557077	1448823
OC saving	0%	2.86%	3.57%	9.94%	16.20%
TAC \$/year	2859573	2773354	2748707	2580672	2424471
TAC saving	0%	3.02%	3.88%	9.75%	15.22%

Although it can be inferred that the increase of methanol mass fraction in product can decrease the separation difficulty in C3, and can lead a decrease of energy and capital cost. The influence of methanol fraction on cost is even greater than that of acetone fraction. With the product methanol mass fraction varied from 300 ppm to 500 ppm, the reboiler duty of C3 is decreased by 53.04% and the total energy cost, total

capital cost and TAC of the process are decreased by 16.22%, 13.71% and 15.22%, respectively, which indicated that the decrease of product purity on methanol fraction scale is of more potential on energy saving.

5. CONCLUSION

In this paper, a typical three column acetone refining distillation sequence model was established and optimized. Seven different heat integration schemes using heat recovery from column top vapor and hot water from other sections were applied and compared with the typical process. All the structures were optimized using TAC optimization, and the cost are compared. The main conclusions can be summarized as follows:

1) Heat integration technology can decrease the energy and capital cost significantly, especially for S1b and S3b schemes. S3b with 17.16% reduction on TAC can achieve largest energy and TAC saving percentage. S1b with simpler structure and 16.90% reduction on TAC which has similar energy/cost saving behaviors is more recommend for industrial application due to safety and control concerns.

2) The decrease of product purity can decrease the TAC cost. With the mass fraction of acetone decrease from 99.9% to 99.7%, the TAC can be saved by 3.88%. With the mass fraction of methanol increase from 300 ppm to 500 ppm, the TAC can be saved by 15.22%. The TAC saving differences indicated that the amount of methanol in product has a much higher influence on process cost rather than acetone mass fraction.

3) The optimized structures with different product purities is also suitable for heat integration, which indicated that the energy consumption and TAC can achieve further reduction via the combination of the two schemes.

4) The results differences from the purity analysis indicated that the membrane or molecular sieve research based on water/acetone separation or water/cumene/acetone separation should take more concerns on the selectivity on trace amount of methanol since it has a larger influence on process separation difficulty.

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